

Author index

- Adair, J.R. 703
 Adiwinata, J. 443
 Alakhov, V.Yu. 39
 Anand, N.N. 541
 Appelhans, H. 215
 Arakawa, T. 721
 Argos, P. 461, 565
- Badalov, P.R. 453
 Balaram, P. 95
 Baldrich, M. 563
 Balland, A. 629
 Ballery, N. 199
 Bates, P.A. 13
 Beato, M. 61
 Betton, J.-M. 5, 55, 199
 Betzel, Ch. 161
 Billetta, R. 531
 Bleasby, A.J. 153
 Bott, R. 649
 Boulain, J.-C. 139
 Bowen, D.J. 515
 Britt, K.A. 523
 Bundle, D.R. 541
- Calogero, R. 133
 Caracci, L. 509
 Castiglia, D. 531
 Celano, B. 133
 Chaidaroglou, A. 127
 Chait, B.T. 29
 Chang, C.-H. 583
 Chang, G. 611
 Chirgadze, Yu. 105
 Chou, K.-C. 509
 Clark-Lewis, I. 29
 Clemen, A. 215
 Creaser, E.H. 523
- Daggett, V. 677
 Davies, P.L. 145
 de Haas, G.H. 599
 Delarue, M. 461
 Desmadril, M. 199
 Dijkman, R. 599
 Dodson, G.G. 635
 Dott, K. 629
 Dubuc, G. 541
 Ducancel, F. 139
 Dumler, I.L. 453
- Efimov, A.V. 411
 Eigenbrot, C. 591
 Engh, R.A. 469
 Eroshkin, A.M. 425
- Fairbrother, W.J. 5
 Fedorov, O.V. 411
 Fendly, B.M. 547
 Field, H. 641
 Finkelstein, A.V. 1
 Fischel-Ghodsian, F. 577
 Fisher, K.L. 547
 Fol, B. 173
 Fomin, V.I. 425
 Ford, C. 193
 Fothergill, J.E. 235
 Fox, G.M. 721
 Frane, J. 649
 Fujimura, T. 443
 Fukui, T. 713
 Furukawa, K. 691, 733
 Furuta, R. 713
- Garnovskaya, M.N. 453
 Gavel, Y. 433
 Gidney, M.A.J. 541
 Goebel, W. 563
 Go, N. 393
 Gonzalez, F.J. 571
 Goodfellow, J.M. 419, 495
 Goraj, K. 259
 Gorman, C.M. 547
 Grandgeorge, M. 629
 Gray, P.M.D. 235
 Gualerzi, C.O. 133
 Gudkov, A.T. 709
 Gullick, W.J. 245
 Gurevich, V.V. 453
- Hakoshima, T. 443
 Hall, L. 5, 55, 199, 515
 Handel, T. 233
 Hanioka, N. 571
 Hansen, D.E. 69
 Harutyunyan, E.H. 161
 Hauss, C. 629
 Hayakawa, T. 49
 Hemminki, A. 181
 Hew, C.L. 145
 Hibino, T. 449
 Hill, C.P. 635
 Holbrook, S.R. 659, 667
 Holm, L. 181, 403
 Hori, K. 273
 Huang, P.C. 205
 Huber, R. 469
 Hunt, P.D. 635
- Ikehara, M. 49, 443
 Islam, S.A. 13
- Janin, J. 1
 Jansoni, J.N. 173
 Jansson, B. 555
- Kaartinen, M. 403
 Kabanov, A.V. 39
 Kamiya, S. 725
 Kantrowitz, E.R. 127
 Karplus, M. 673
 Kawai, H. 85
 Kawashima, H. 713
 Kemp, G.J.L. 235
 Kent, S.B.H. 29
 Kerver, J. 599
 Kikuchi, T. 85
 Kim, C.-S. 725
 Kim, S.-H. 659, 667
 King, D.J. 703
 Kirsch, J.F. 625
 Kirschner, K. 249
 Kito, M. 725
 Knowles, J.K.C. 181, 403
 Kobayashi, M. 393
 Kobayashi, Y. 393
 Koivula, A.K. 181
 Kojima, S. 527
 Kollman, P.A. 677
 Korzekwa, K. 571
 Kossiakoff, A.A. 591
 Kotani, H. 713
 Koyama, S. 393
 Kuipers, O.P. 599
 Kulichkov, V.A. 425
 Kumagai, I. 449, 527
- Kurochkina, N. 105
 Kyogoku, Y. 267, 393
- La Teana, A. 133
 Laaksonen, L. 403
 Larimer, F.W. 227
 Lawn, R.M. 547
 Lecocq, J.-P. 629
 Lee, K.S. 205
 Lehtovaara, P.M. 181
 Lepage, P. 629
 Levashov, A.V. 39
 Littlechild, J.A. 515
 Livingston, D.J. 111, 117
 Luger, K. 249
 Lyons, A. 703
- MacKenzie, C.R. 541
 Maeda, H. 691, 733
 Mandal, S. 541
 Mandecki, W. 221
 Mantafounis, D. 605
 Markland, W. 111, 117
 Marks, B.J. 547
 Martial, J.A. 259
 Mathiowitz, G. 577
 Matsuo, H. 267
 Matsuo, N. 713
 McCray, G. 547
 McElroy, H.E. 43
 McGinley, M. 721
 McGregor, M.J. 13
 Meckelein, B. 215
 Mehler, E.L. 415
 Ménez, A. 139
 Meulien, P. 629
 Miller, S. 77
 Millican, A. 703
 Minard, P. 5, 55, 199, 515
 Mischler, F. 629
 Missiakas, D. 5, 55
 Miura, K. 449, 527
 Moras, D. 461
 Morikawa, M. 49
 Morioka, H. 443
 Mouawad, L. 199
 Murali, C. 523
 Mural, R.J. 227
 Murzina, N.V. 709
 Muskal, S.M. 659, 667
- Nakagawa, S. 443
 Nakano, K. 713
 Narang, S.A. 541
 Narhi, L.O. 721
 Natochin, M.Yu. 453
 Nikiforov, T. 215
 Nikonov, S. 105
 Nilsson, B. 555
 Nishida, Y. 49
 Nishikawa, S. 49, 443
- Oda, M. 733
 Ohkubo, T. 393
 Ohue, M. 713
 Okamoto, Y. 85
 Owens, R.J. 703
- Paborsky, L.R. 547
 Palmcrantz, C. 555
 Paton, N.W. 235
 Perahia, D. 199
 Perry, L.J. 611
- Peters, I.D. 145
 Peter, W. 61
 Phipps, J. 541
 Pitts, J. 605
 Planas, A. 625
 Poch, O. 461
 Pollock, D. 111, 117
 Pon, C.L. 133
 Powell, M.J. 69
- Ramakrishnan, C. 95
 Randal, M. 591
 Rees, A.R. 641
 Reilly, P.J. 193
 Renard, A. 259
 Rhee, I.-K. 205
 Robertus, J.D. 43
 Rohde, M.F. 721
 Rooman, M.J. 23
- Saenger, W. 161
 Santi, D.V. 95
 Saqi, M.A.S. 419
 Sato, A. 393
 Sato, T. 725
 Sattentau, Q.J. 13
 Schiffer, M. 583
 Schlagenhauf, E. 173
 Schuster, S.M. 739
 Serikawa, Y. 267
 Shinshi, H. 733
 Shirakawa, M. 267
 Shirokova, E.P. 453
 Shmukler, B.E. 453
 Shoichet, B. 95
 Sierks, M.R. 193
 Sinnott, B. 541
 Smith, T.F. 577
 Sollazzo, M. 531
 Soper, T.S. 227
 Sowdhamini, R. 95
 Spurio, R. 133
 Srinivasan, N. 95
 Sternberg, M.J.E. 13, 245
 Straub, J.E. 673
 Suske, G. 61
 Svensson, B. 193
 Szadkowski, H. 249
- Taira, K. 691, 733
 Takasaki, Y. 273
 Takeda, S. 449
 Tanaka, T. 49, 443
 Tate, K.M. 547
 Teeri, T.T. 403
 Teplyakov, A.V. 161
 Thanki, N. 495
 Thornton, J.M. 23, 479, 495
 Tolley, S.P. 635
 Tomita, K. 443
 Tordo, N. 461
 Tramontano, A. 531
 Trémeau, O. 139
- Uchida, E. 49
 Uebayasi, M. 691
 Uemura, H. 49
 Uesugi, S. 49, 443
 Uhlén, M. 555
 Utsumi, S. 725
- Van Heeke, G. 739
 van Meersbergen, J. 599

Author index

Vehar, G.A. 547
Veilleux, C. 611
Verheij, H.M. 599
Vingron, M. 565
Visger, J.V. 721
Vis, R. 599
von Heijne, G. 433

Ward, R.J. 635
Watson, H.C. 515
Wetzel, R. 611

Whittle, N.R. 703
Williams, R.J.P. 5
Wilmanns, M. 173
Wilmot, C.M. 479
Wilson, K.S. 161
Wodak, S.J. 23
Woo, D.D.L. 29
Wootton, J.C. 153
Wright, H.T. 469

Xu, Z.-B. 583

Yamada, M. 713
Yamada, Y. 49
Yamagishi, J. 713
Yamayoshi, M. 713
Yarranton, G.T. 641, 703
Yon, J.M. 5, 55, 199
Young, N.M. 541

Zanetti, M. 531
Zhilkin, P.A. 425
Zozulya, S.A. 453
Zvyaga, T.A. 453

Subject index

AIDS

HIV binding domains, CD4 antigen, human, three-dimensional structure 13

Alcohol dehydrogenase

yeast, substrate pocket amino acid changes 523

Aldolase C

rat, expression plasmids construction/bacterial expression/hybrid formation, *Escherichia coli* 273

Alkaline phosphatase

Escherichia coli, active site, role—aspartate 101, site-directed mutagenesis 127

Amino acid sequence templates

local folding motifs, protein structure prediction 23

Amino acid side chains

serine/threonine/tyrosine residues, hydration, secondary protein structure effects on 495

Amino acid substitution

free energy changes 419

Amino acids

surface exposure, prediction from protein sequence 659

α -Amylase

Bacillus stearothermophilus, structure/function, random mutagenesis 181

Anti-thyroglobulin antibody

idiotypic determinant Id62, expression, mouse 531

Antibodies

site-specific labelling, surface cysteine residues 703

Antibody production

tissue factor, transient expression, mammalian cells 547

Antifreeze proprotein

Pseudopleuronectes americanus, biosynthesis, *Escherichia coli* 145

Asparagine synthetase

human, expression, *Saccharomyces cerevisiae* 739

Aspergillus awamori

glucoamylase, catalytic mechanism, Asp176/Glu179/Glu180 mutagenesis 193

Bacillus stearothermophilus

α -amylase, structure/function, random mutagenesis 181

Bacterial expression

aldolase C, *Escherichia coli* 273

immunoglobulins, light/heavy chain variable regions, *Escherichia coli* 641

α -lactalbumin, goat, *Escherichia coli* 449

monoclonal antibody, murine λ_1 chain, *Escherichia coli* 541

protein A—neurotoxin fusion protein, *Escherichia coli* 139

protein A, deletion mutants, gene fusion system, *Escherichia coli* 555

rabbit uteroglobin, *Escherichia coli* 61

α/β Barrel protein

de novo design 233

octarellin, synthesis/purification/structure 259

protein folding 249

Bimolecular complex formation

entropy 1

CD4 antigen

human, HIV binding domains, three-dimensional structure 13

Catalytic antibodies

enzyme design 69

Chemical synthesis

human transforming growth factor- α 29

Chymosin

catalysis, optimum pH, modification 605

Crystal structure

IGP synthase, recombinant synthase domain, *Escherichia coli* 173

γ -Crystallin

eye lens, calf, molecular cartography 105

Cysteine

disulphide-bonding state, prediction, computer-simulated neural networks 667

Cytochrome P450

IIA1/IIA2, catalytic activity, sequence requirements 571

DNA polymerase

structure, sequence similarities 461

Database

object-oriented, protein modelling/protein structure 235

validated, non-redundant composite protein sequence, construction 153

Dimeric proteins

subunit interfaces, structure 77

Disulfide bond

stereochemistry, site-directed mutagenesis, computer modelling 95

Electrostatic effects

proteins, simulation, dielectric response models 415

Enkephalin

three-dimensional structure, Monte Carlo simulated annealing 85

Enzyme design

catalytic antibodies 69

Escherichia coli

alkaline phosphatase, active site, role—aspartate 101, site-directed mutagenesis 127

flagellin, protein modelling/supramolecular structures 411

IGP synthase, recombinant synthase domain, crystal structure 173

initiation factor IF1, site-directed mutagenesis, ribosomal

binding/recycling 133

penicillin G acylase, expression/purification/crystallization 635

protein A—neurotoxin, bacterial expression 139

rabbit uteroglobin expression 61

Expression plasmids

aldolase C, rat, construction 273

Eye lens

calf, γ -crystallin, molecular cartography 105

Factor IX

recombinant, position +1 alanine substitution, effects on biological activity 629

Flagellin

Escherichia coli, protein modelling/supramolecular structures 411

Free energy changes

amino acid substitution 419

Fusion protein

antifreeze proprotein, *Pseudopleuronectes americanus*, biosynthesis, *Escherichia coli* 145

protein A—neurotoxin, bacterial expression, *Escherichia coli* 139

tissue factor, transient expression, mammalian cells 547

GAL4 protein

yeast, DNA binding domain, characteristics 267

Gene duplication

plasminogen activator, tissue-type, interdomain interactions 111

Gene library

open reading frames, randomized, construction 221

Glucoamylase

Aspergillus awamori, catalytic mechanism, Asp176/Glu179/Glu180 mutagenesis 193

Glycinin

soybean, functional properties/nutritional value, improvement, protein engineering 725

Glycoproteins

N-glycosylation, statistical study 433

Growth factor receptors

transmembrane sequence, α -helix dimerization 245

Histidine decarboxylase

Lactobacillus 30a, site-directed mutagenesis 43

HIV

binding domains, CD4 antigen, human, three-dimensional structure 13

α -Human atrial natriuretic polypeptide

conformation, comparison—Met(O)- α -hANP, NMR spectroscopy 393

Human growth hormone

artificial mutant variants, structure/activity 49

IGP synthase

Escherichia coli, recombinant synthase domain, crystal structure 173

Immunoglobulins

anti-2-phenyloxazolone IgG, O λ 1 idiotype, somatic variant/variable domains, computer-aided modelling, mouse 403

anti-thyroglobulin antibody, idiotypic determinant Id62, expression, mouse 531

light-chain dimers, structure, simulated annealing, X-PLOR 583

Subject Index

- light/heavy chain variable regions, mouse, expression, *Escherichia coli* 641
- monoclonal antibody, murine λ_1 chain, synthesis/expression, *Escherichia coli* 541
- Initiation factor IF1**
Escherichia coli, site-directed mutagenesis, ribosomal binding/recycling 133
- Insertion mutagenesis**
metallothionein, domain spacing 205
- Interferon- γ**
human, C-terminus, mutational analysis 611
- α -Lactalbumin**
goat, expression/refolding, *Escherichia coli* 449
- Lactobacillus* 30a**
histidine decarboxylase, site-directed mutagenesis 43
- Lipid anchors**
attachment, water-soluble proteins 39
- Metallothionein**
domain spacing, insertion mutagenesis 205
- Microbial expression**
asparagine synthetase, human, *Saccharomyces cerevisiae* 739
- Monoclonal antibody**
murine λ_1 chain, synthesis/expression, *Escherichia coli* 541
- Monte Carlo simulated annealing**
enkephalin, three-dimensional structure 85
- Mucus proteinase inhibitor**
human, inhibitory specificity, location 215
- NMR spectroscopy**
 α -human atrial natriuretic polypeptide, conformation, comparison—Met(O)- α -hANP 393
phosphoglycerate kinase, yeast, structural domains 5
- Octarellin**
synthesis/purification/structure 259
- Oligonucleotide cassette mutagenesis**
asparagine synthetase, human 739
- Open reading frames**
randomized, construction 221
- Pancreatic phospholipase A₂**
porcine, catalytic activity, residue 31 size/polarity effects on 599
- Pancreatic trypsin inhibitor**
basic, C30A/C51A mutant, X-ray structure 591
- Penicillin G acylase**
Escherichia coli, expression/purification/crystallization 635
- anti-2-Phenylloxazalone IgG**
Ox1 idiotype, somatic variant/variable domains, computer-aided modelling, mouse 403
- Phosphoglycerate kinase**
yeast, ATP binding site, site-directed mutagenesis 515
yeast, conformational probes, internal cysteines 199
yeast, site-directed mutagenesis, structural domains, expression/characterization 55
yeast, structural domains, NMR spectroscopy 5
- Plasmids**
artificial-ribozyme-releasing, construction 733
- Plasminogen activator**
tissue-type, structure—function analysis, mutagenesis 117
tissue-type, interdomain interactions 111
- Protection—modification**
sulphydryl group derivatization, multi-cysteine proteins 625
- Protein A**
deletion mutants, expression/purification, gene fusion system, *Escherichia coli* 555
- Protein conformation**
pancreatic trypsin inhibitor, basic, disulphide bridge removal effects on 591
- Protein crystallization**
penicillin G acylase, *Escherichia coli* 635
- Protein engineering**
alcohol dehydrogenase, yeast, substrate pocket amino acid changes 523
ATG vectors 227
 α/β barrel protein, *de novo* design 233
chymosin, catalysis optimum pH modification 605
flagellin, *Escherichia coli*, supramolecular structures 411
glycinin, soybean, functional properties/nutritional value improvement 725
glycoproteins, N-glycosylation 433
human transforming growth factor- α , chemical synthesis/purification/characterization 29
- phosphoglycerate kinase, yeast, ATP binding site, site-directed mutagenesis 515
- plasminogen activator, tissue-type, structure—function analysis 117
- plasminogen activator, tissue-type, interdomain interactions 111
- vaccines, variable fragments databank 425
- Protein folding**
 α/β barrel protein 249
 α -lactalbumin, goat, refolding 449
octarellin, α/β barrel protein 259
phosphoglycerate kinase, yeast, NMR spectroscopy 5
phosphoglycerate kinase, yeast, conformational probes, internal cysteines 199
phosphoglycerate kinase, yeast, structural domains 55
tumour necrosis factor- α , human, analogue/native protein, comparison 721
- Protein modelling**
anti-2-phenylloxazalone IgG, Ox1 idiotype, somatic variant/variable domains, mouse 403
object-oriented database 235
 α_1 -proteinase inhibitor, intact form, molecular dynamics 469
- Protein sequence**
validated, non-redundant composite, database, construction 153
- Protein sequence alignment**
dynamic programming, STRALIGN 577
reliable regions, determination 565
- Protein structure**
amino acids surface exposure, prediction from protein sequence 659
 γ -crystallin, eye lens, calf, molecular cartography 105
cysteine disulphide-bonding state, prediction, computer-simulated neural networks 667
dimeric proteins/tetrameric proteins, subunit interfaces 77
DNA polymerase/RNA polymerase, sequence similarities 461
enkephalin, Monte Carlo simulated annealing 85
HIV binding domains, CD4 antigen, human 13
immunoglobulins, light-chain dimers, simulated annealing, X-PLOR 583
object-oriented database 235
prediction, amino acid sequence templates, local folding motifs 23
secondary, dynamic programming, STRALIGN 577
secondary, effects on serine/threonine/tyrosine residues hydration 495
secondary, prediction, β -turns 479
tertiary, X-ray crystallography, statistical analysis 649
- Protein translocation**
water-soluble proteins, lipid anchors attachment 39
- Proteinase K**
three-dimensional structure, comparison—thermitase, X-ray structure 161
- α_1 -Proteinase inhibitor**
intact form, modelling, molecular dynamics 469
- Proteins**
electrostatic effects, simulation, dielectric response models 415
water-soluble, lipid anchors attachment/membrane transport 39
- Pseudopleuronectes americanus***
antifreeze proprotein, biosynthesis, *Escherichia coli* 145
- RNA cleavage**
ribozymes, energetics/mechanism of action 691
- RNA polymerase**
structure, sequence similarities 461
- Random mutagenesis**
 α -amylase, *Bacillus stearothermophilus*, structure/function 181
interferon- γ , human, C-terminus 611
- Rhodopsin**
functional expression *in vitro*/site-directed mutagenesis, bovine 453
- Ribonuclease T1**
thermostable mutant, preparation/characterization 443
- Ribozymes**
artificial-ribozyme-releasing plasmids, construction 733
RNA cleavage, energetics/mechanism of action 691
- Site-directed mutagenesis**
alkaline phosphatase, *Escherichia coli*, active site, role—aspartate 101 127
anti-thyroglobulin antibody, idiotypic determinant Id62, mouse 531
chymosin, catalysis optimum pH modification 605
cysteine residue modification, multi-cysteine proteins 625
disulphide bond stereochemistry, computer modelling 95
histidine decarboxylase, *Lactobacillus* 30a 43
initiation factor IF1, *Escherichia coli*, ribosomal binding/recycling 133
interpretation, linear free energy relations, Brønsted plots 673

- pancreatic phospholipase A₂, porcine, residue 31, effects on catalytic activity 599
- phosphoglycerate kinase, yeast, ATP binding site 515
- phosphoglycerate kinase, yeast, conformational probes, internal cysteines 199
- phosphoglycerate kinase, yeast, structural domains, expression/characterization 55
- rhodopsin, bovine, 453
- subtilisin inhibitor, *Streptomyces*, reaction site P4, effects on inhibitory activity 527
- Site-specific mutagenesis**
 - antibodies, surface cysteine residues, radiolabelling 703
 - rapid method 563
- Snake toxins**
 - protein A-neurotoxin fusion protein, bacterial expression, *Escherichia coli* 139
- Soybean**
 - glycinin, functional properties/nutritional value, improvement, protein engineering 725
- Streptomyces***
 - subtilisin inhibitor, reaction site P4, site-directed mutagenesis, effects on inhibitory activity 527
- Subtilisin inhibitor**
 - Streptomyces*, reaction site P4, site-directed mutagenesis, effects on inhibitory activity 527
- Tetrameric proteins**
 - subunit interfaces, structure 77
- Thermitase**
 - three-dimensional structure, comparison—proteinase K, X-ray structure 161
- Tissue factor**
 - transient expression, mammalian cells 547
- Transforming growth factor- α**
 - human, chemical synthesis/purification/characterization 29
- Triosephosphate isomerase**
 - active site mutants, molecular dynamics simulations 677
- Tumour necrosis factor- α**
 - human, structure—activity relationships 713
 - human, structure, analogue/native protein, comparison 721
- β -Turns**
 - nomenclature/prediction 479
- Tyrosine kinase**
 - growth factor receptors, transmembrane sequence, α -helix dimerization 245
- Uteroglobin**
 - rabbit, expression, *Escherichia coli* 61
- Vaccines**
 - protein engineering, variable fragments databank 425
- Vectors**
 - ATG, protein engineering 227
- X-ray crystallography**
 - protein structure, tertiary, statistical analysis 649
- X-ray structure**
 - proteinase K/thermitase, comparison 161
- Yeast**
 - alcohol dehydrogenase, substrate pocket amino acid changes 523
 - GAL4 protein, DNA binding domain, characteristics 267
 - phosphoglycerate kinase, ATP binding site, site-directed mutagenesis 515
 - phosphoglycerate kinase, conformational probes, internal cysteines 199
 - phosphoglycerate kinase, site-directed mutagenesis, structural domains, expression/characterization 55
 - phosphoglycerate kinase, structural domains, NMR spectroscopy 5